3H-1,2-Dithiole-3-thione, 4-methyl-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.47

Global applicability domain: Inside

Local applicability domain index: 9.28e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

Image not found
Hexamethylbenzene
Measured: 6.31
Predicted: 5.75

Image not found
1,4-Dibromobenzene
Measured: 5.21
Predicted: 5.09

Image not found
Naphthalene
Measured: 5.19
Predicted: 5.07

Image not found
1,3,5-Trichlorobenzene
Measured: 4.85
Predicted: 5.06

Image not found
1,2,3,4-Tetrachlorobenzene
Measured: 5.64
Predicted: 5.76